The Role of Supercomputing in Developing Fuels for Next Generation Nuclear Reactors

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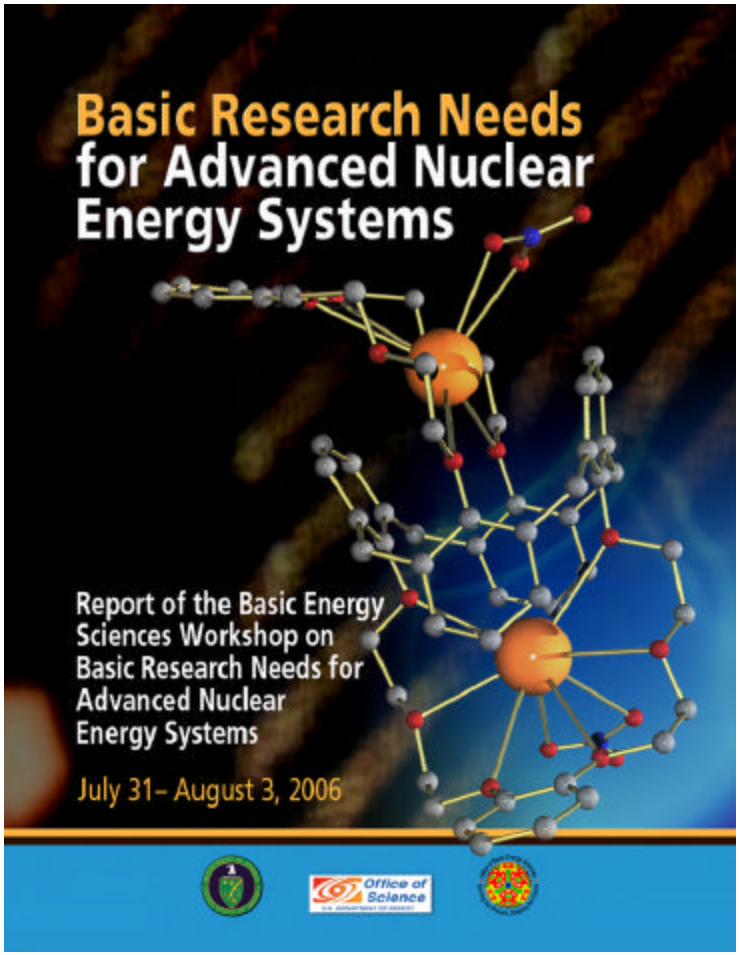
What do We Want from an Advanced Nuclear Energy System (ANES) ?

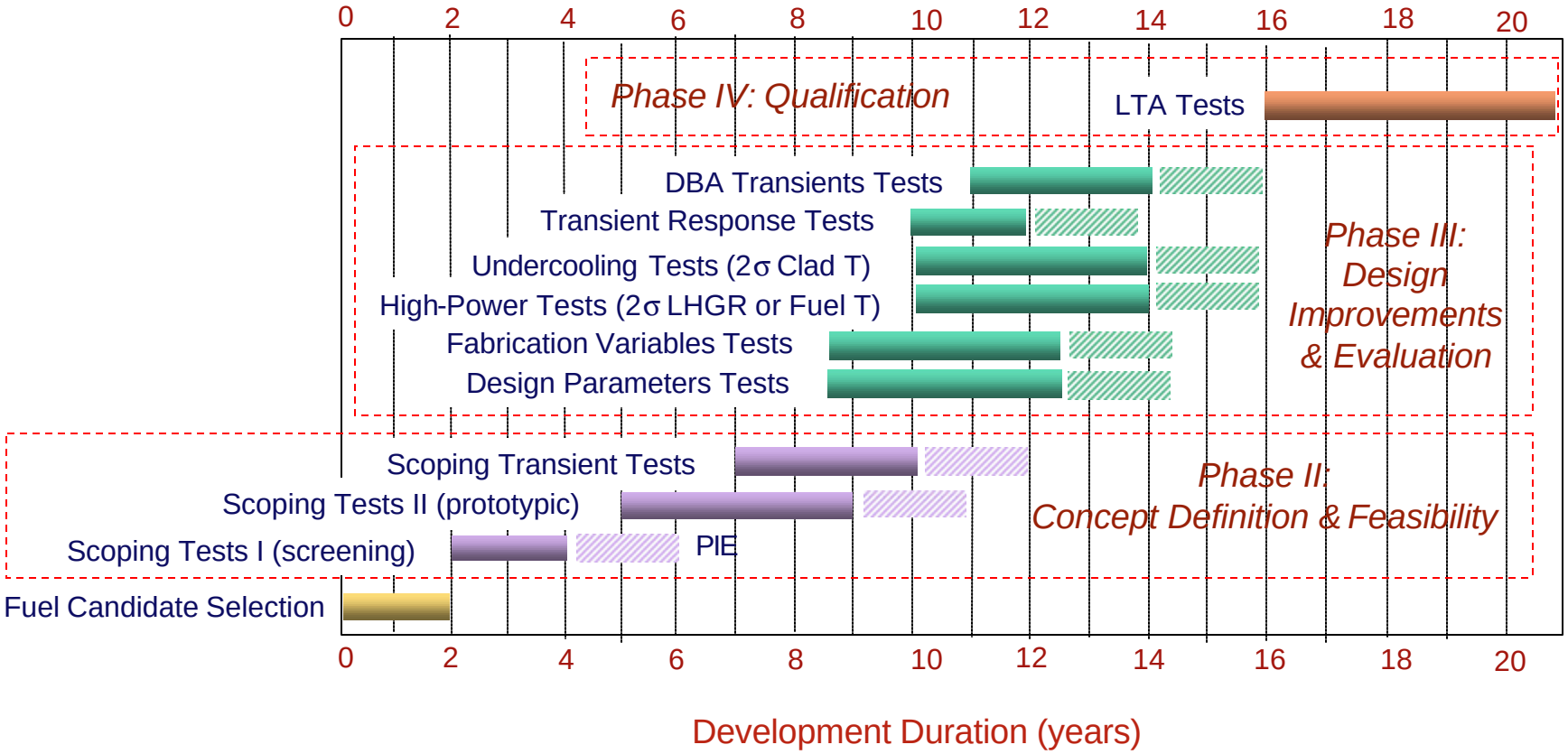
- Reduced Waste
- Maximize Energy Content Utilization of Fuel
- Increased Safety
- Improved Operational Efficiency

These desires require new fuel systems with long lifetimes in extreme environments.



Qualification of a New Nuclear Fuel Currently Takes 20 Years

Source: K. Pasamehmetoglu, D. Crawford
GNEP Fuel Development Road Map



Fuel Qualification Timeline is Controlled by Reactor Residence Times

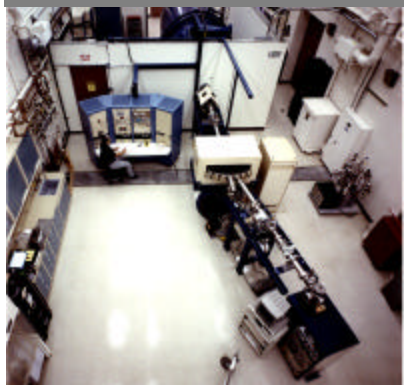
- Twenty year process is for a fuel element with a 4.5 year reactor lifetime (3 x 1.5 year cycles)
  - Development process is dominated by Advanced Test Reactor exposures and Post Irradiation Examinations
  - Engineering endeavor with the fuel science limited to the first 5 years

- A qualified fuel performance code is required with the fuel license application
  - Quantifies of understanding of fuel package behavior during normal operating conditions and design basis accidents (loss of coolant)
    - Documented solution methods
    - Validated constitutive models in operation window

To shorten development times a new process involving advanced scientific computing is needed qualify fuel that breaks reactor exposure bottleneck

Credibility of Qualification Case Relies on our Ability to Capture and Predict Fuel System Behavior in a Wide Range of Conditions

Ion Beam System
~ 50dpa/day



Integrate Experiments & Materials Qualification with ATR & HIFR

Test Reactors
~ 15 dpa/year

Study Behavior of Synthetically-aged Fuel with Post-Irradiation Examination (PIE)

Theoretical Modeling & Numerical Simulations

Multi-Scale Materials Modeling Platforms

Charged particle Irradiations (ions, e^-) & *In Situ* Characterization (TEM, IBA)

Materials Selection & Model Validation

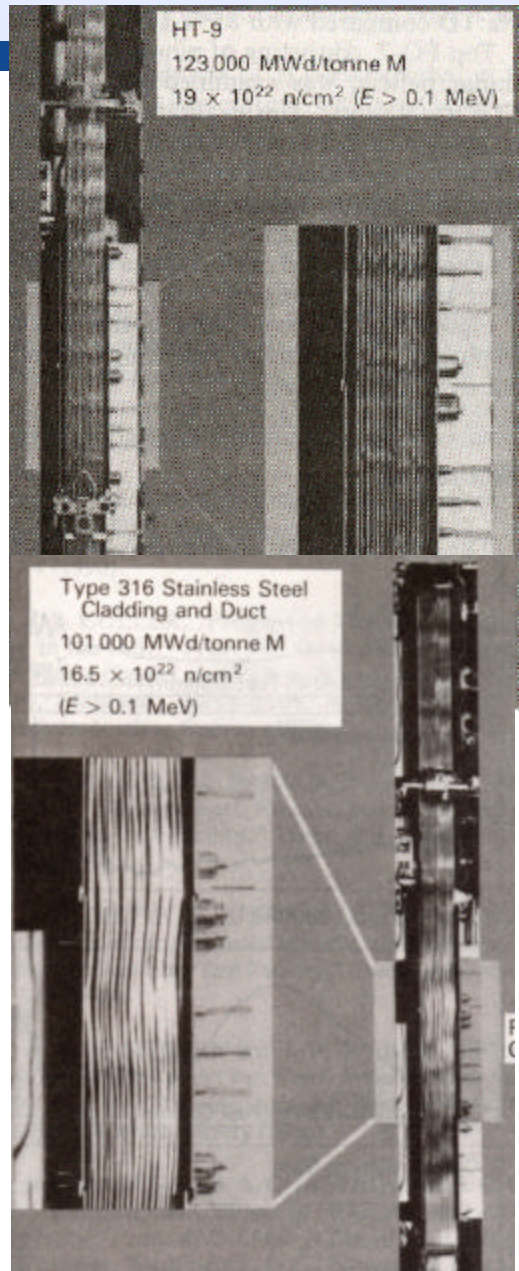
Benchtop Experimentation: TEM, 3D Atom Probe, Diffusion Couples, Laser Flash Thermal Diffusivity

BGL
~ 15 dpa/cpu-week

Fuel Qualification Criteria Remain the Same Regardless of the Sophistication of the Multi-physics Code

- How do predictions of fuel thermal profile (heat generation and transfer) compare to experimental observations as a function of reactor exposure?
- How close does the fuel come to melting during a loss of coolant accident (LOCA) on day one? after six years?
- How closely do fuel depletion simulations capture the evolving chemistry experimentally observed?
- What is the margin to failure of the cladding during a LOCA?
- What mass of actinides and fission products escape into coolant?

Large uncertainties in these fundamental questions will lead NRC to mandate decreased power densities of reactor geometries and shortened fuel element lifetimes

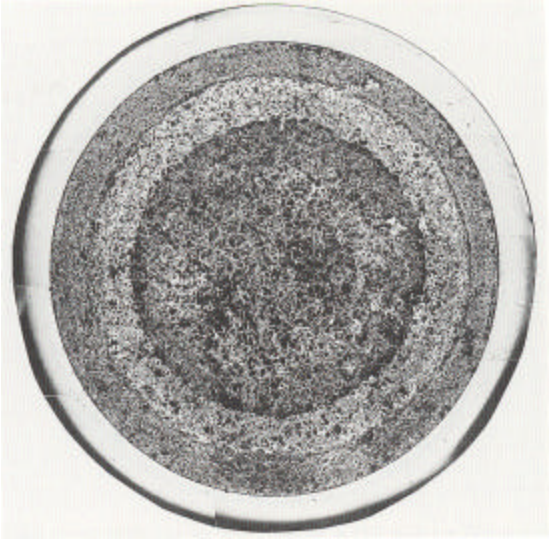


A Wide Array of Constitutive Models are Needed to Bring Closure to Large Scale Multi-physics Codes

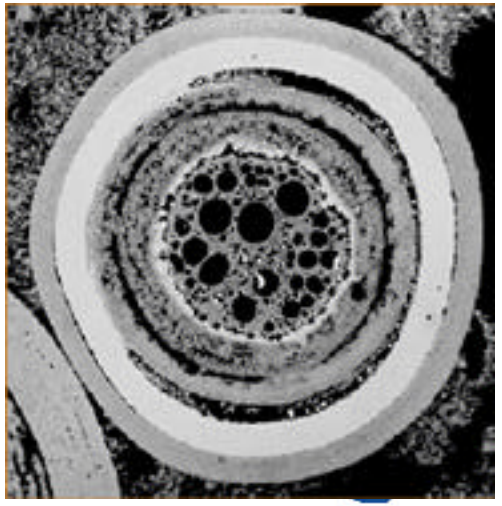
- **Fuel**
  - **Melt temperature as a function of chemistry**
  - **Dimensional stability, heat transfer, and elemental diffusion as a function of chemistry, temperature, and microstructure**
  - **Heat generation due to neutron capture and fission**
  - **Fission product accumulation and gas release**

- **Cladding**
  - **Strength and ductility as a function of microstructure and temperature**
  - **Elemental diffusion of actinides and fission products**
  - **Reaction Chemistry at Interfaces with fluid and fuel leading to thinning**

U-PU-Zr Fast Reactor Fuel

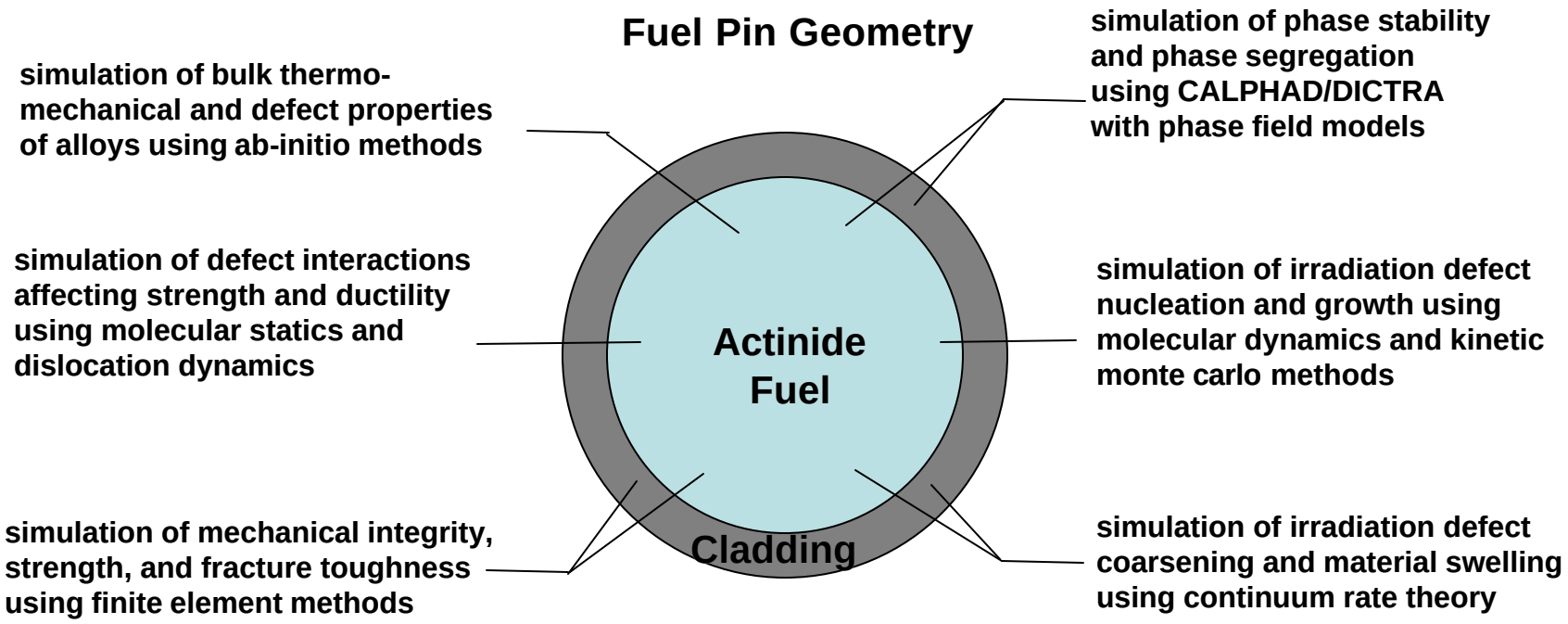


UO_2 TRISO Fuel Particle



The quality and validation pedigree of the models dictate the range of operating conditions for which a fuel will be licensed

Constitutive Model Development Maps onto a Suite of Sub-scale Physics Simulations within a Multi-scale Modeling Program



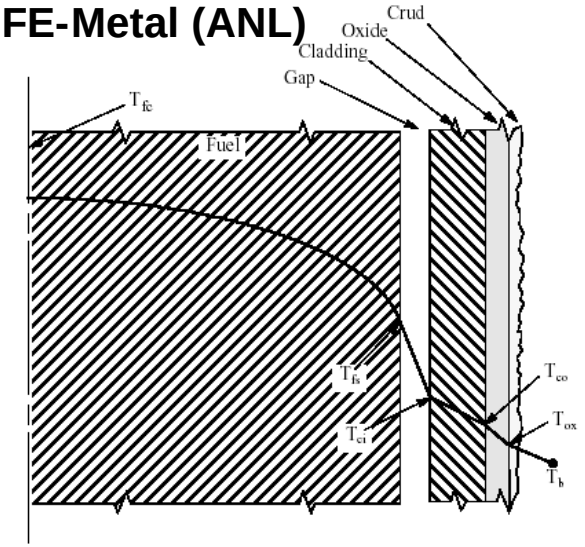
The purpose of a multiscale materials modeling effort is to replace the "burnup" lumped history variable with more meaningful descriptions to increase the regime of applicability of performance models

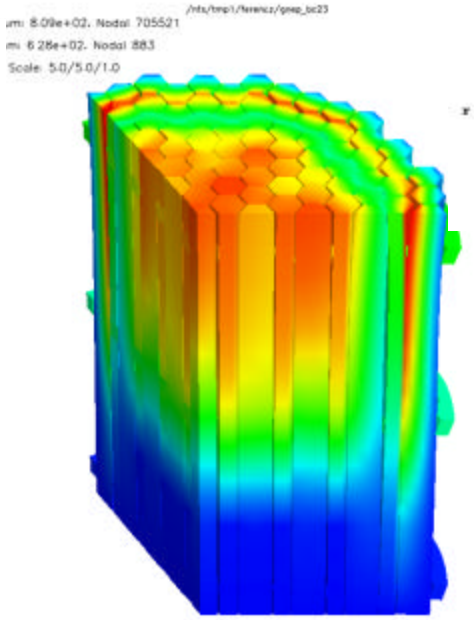
Multi-physics Codes on High Performance Computers (HPC) have the Potential to Increase the Operational Efficiency Nuclear Reactors

- Current fuel performance codes rely on 1.5D simulations using empirical model database obtained from LWR and SFR irradiations
- Lack of geometric and constitutive model complexity yields narrow operational windows

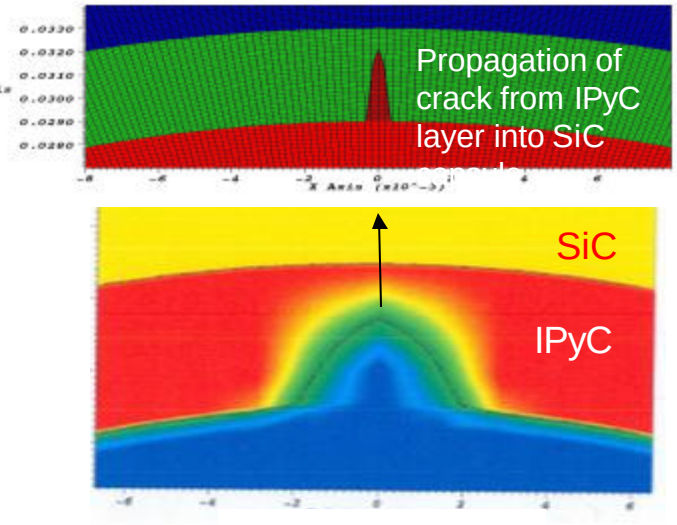
- Exisiting HPC codes can be modified to analyze these systems in full 3D with geometric perturbations and materials variability
- High-throughput for fuel design requires dedicated access to HPC

LIFE-Metal (ANL)





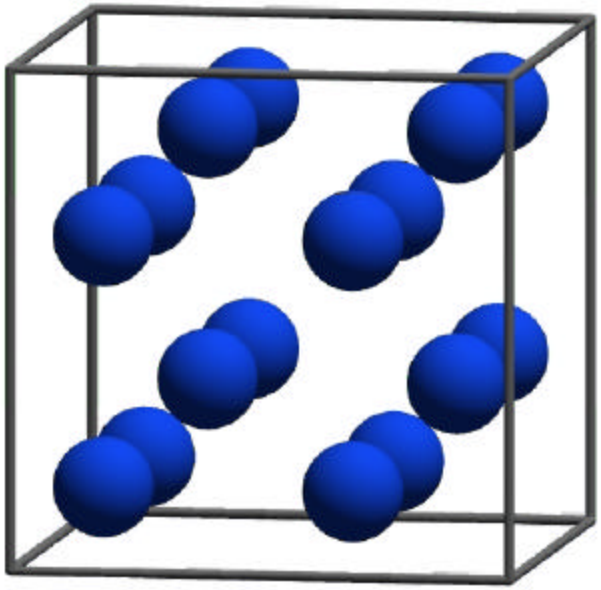
Diablo (LLNL)

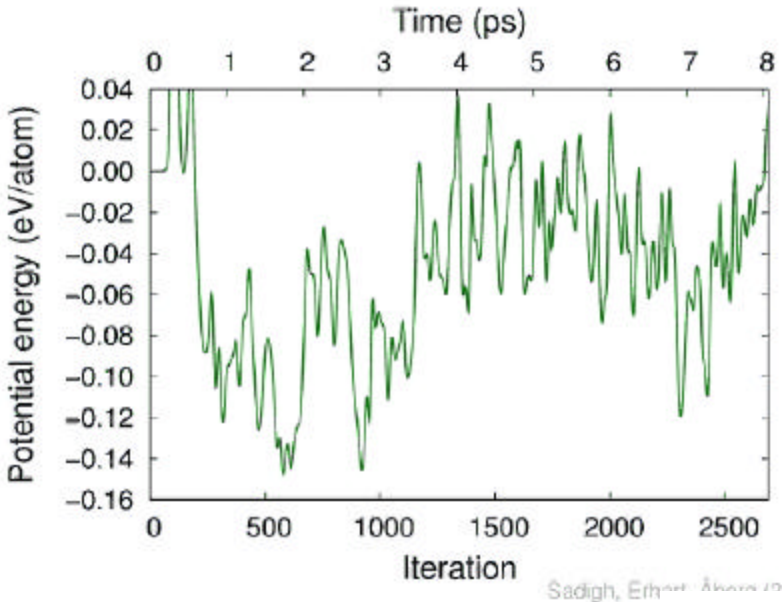


ALE3D (LLNL)

Recent Accomplishments: Discovery of Charge-Density Wave Structures in BCC U

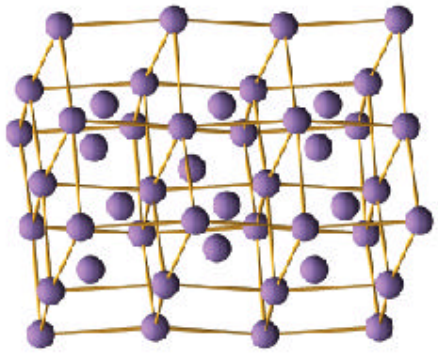
The energy of the bcc phase is lowered by vibrations.





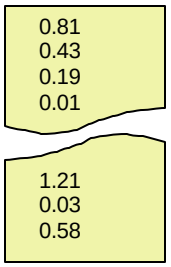
Sadigh, Erhart, Åberg (2009)

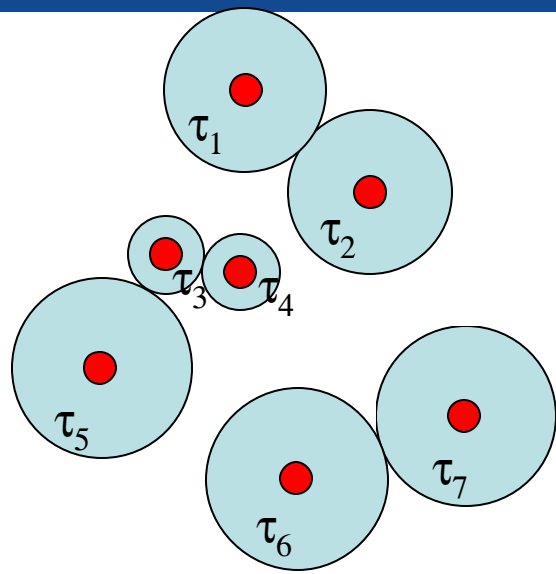
The bcc-U phase is an average of a set of low-energy bcc-related configurations. It is entropically stabilized .

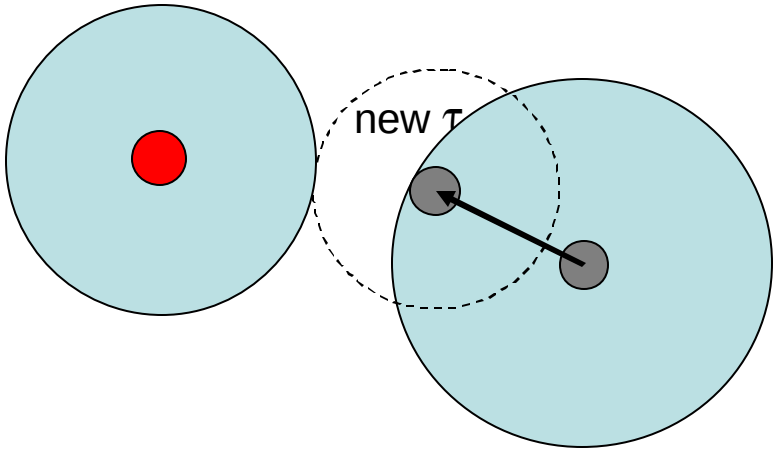


Recent Accomplishments: First-passage Kinetic Monte Carlo Method Developed to Efficiently Simulate Diverse Irradiation Rates

- The first-passage kMC algorithm
  - 1. Construct disjoint protective regions centered on the particles
  - 2. For each walker randomly sample first arrival times from PR-a(t<t) and order them in a time queue $\tau 3 < \tau 4 < \tau 1 < \tau 2 < \tau 7 < \tau 6 < \tau 5$
  - Repeat
    - Find the earliest time in the queue
    - Propagate the particle to boundary
    - Construct a new protective region
    - Pick a new arrival time, insert into the queue
- Efficiency is achieved by scaling the hop distance to the density of diffusers and analytically integrating time spent in protective regions





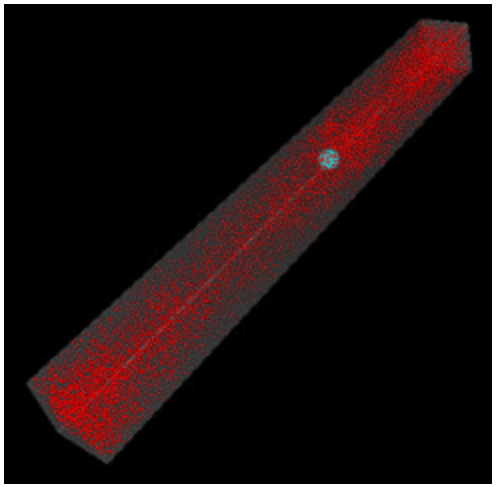


Recent Accomplishments: First-passage Kinetic Monte Carlo Method Developed to Efficiently Simulate Diverse Irradiation Rates

- Simulations of material degradation to high doses under arbitrary dose rates
- New method can be trained with heavy ion irradiation observations and used to extrapolate behavior of materials in reactor conditions

Ion Beam System

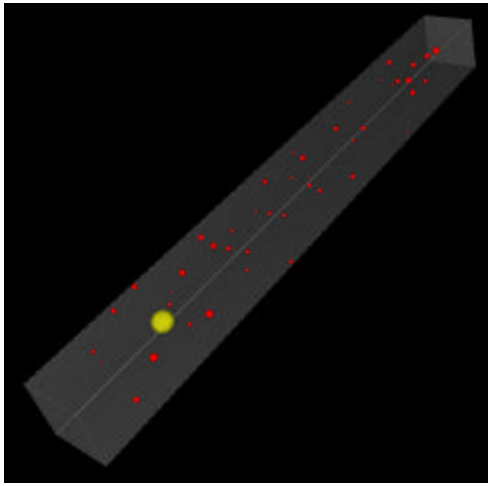
dose rate = 1.5 x10 $^{-4}$ dpa/s



Computational expense = 1.80 dpa / cpu-day
Equivalent irradiation time = 33 hrs

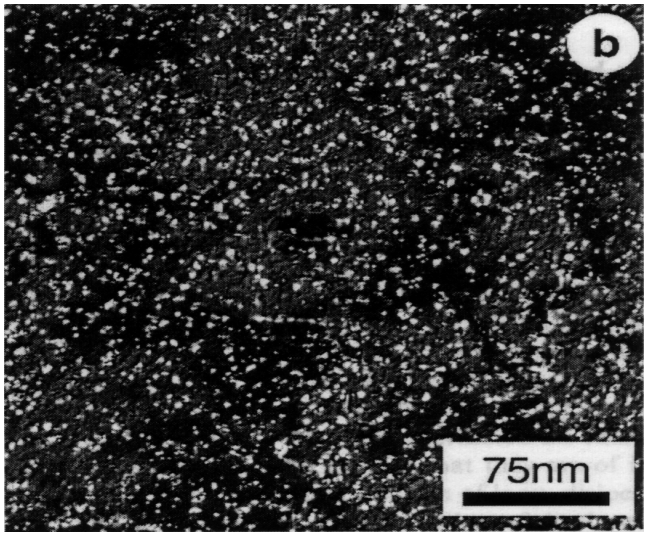
Test Reactor

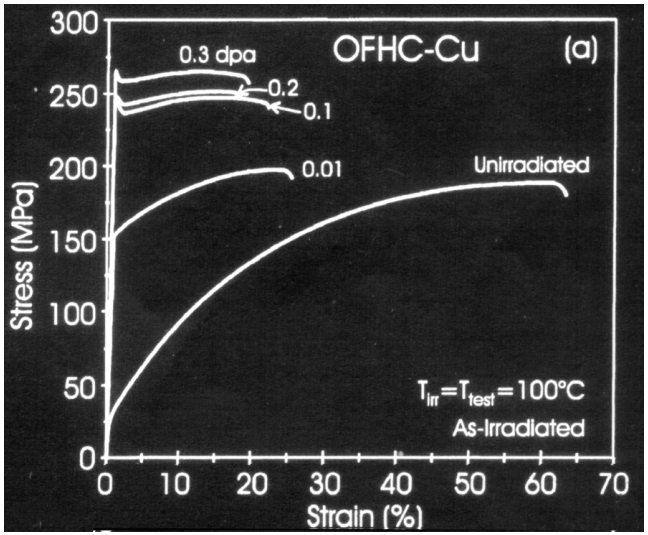
dose rate = 1.5 x10 $^{-8}$ dpa/s



Computational expense = 2.67 dpa / cpu-day
Equivalent irradiation time = 21 years

Debate in the mechanisms of irradiation hardening may be settled by simulation





- Nanometer size defects are induced by the coarsening of nuclear collisions in nuclear core materials
- Defects are at the resolution limit of current electron microscopes
- Defects are known to increase initial strength and decrease ductility
  - Combination leads to a decrease in fracture toughness of engineering components
- Fundamental question of resistance addition
  - Add obstacles

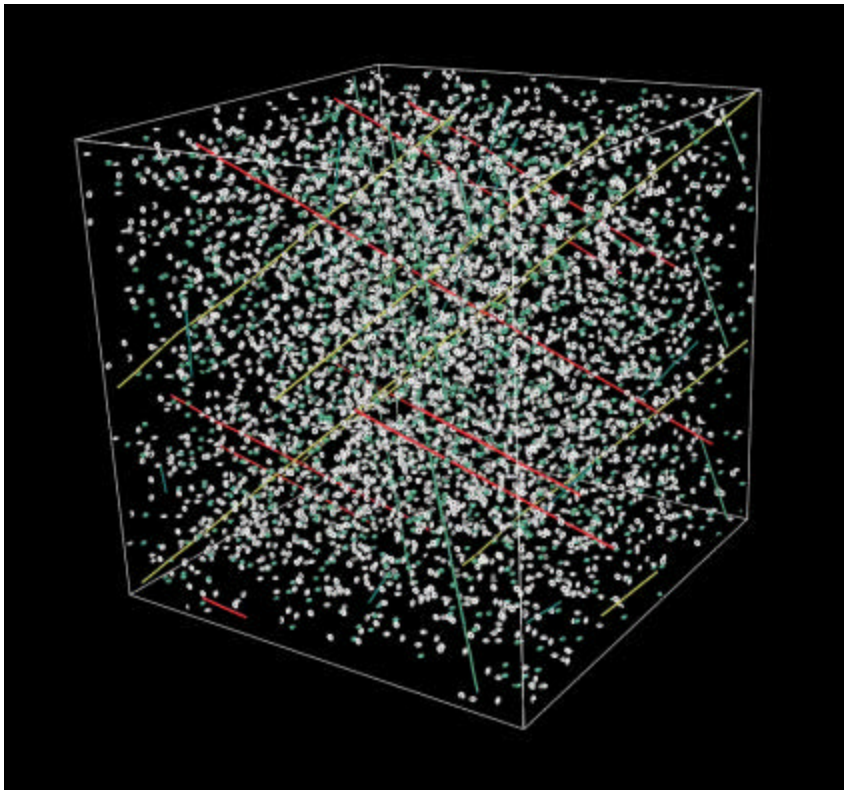
OR $$s = mb\sqrt{a\,r + bN_l d_l}$$

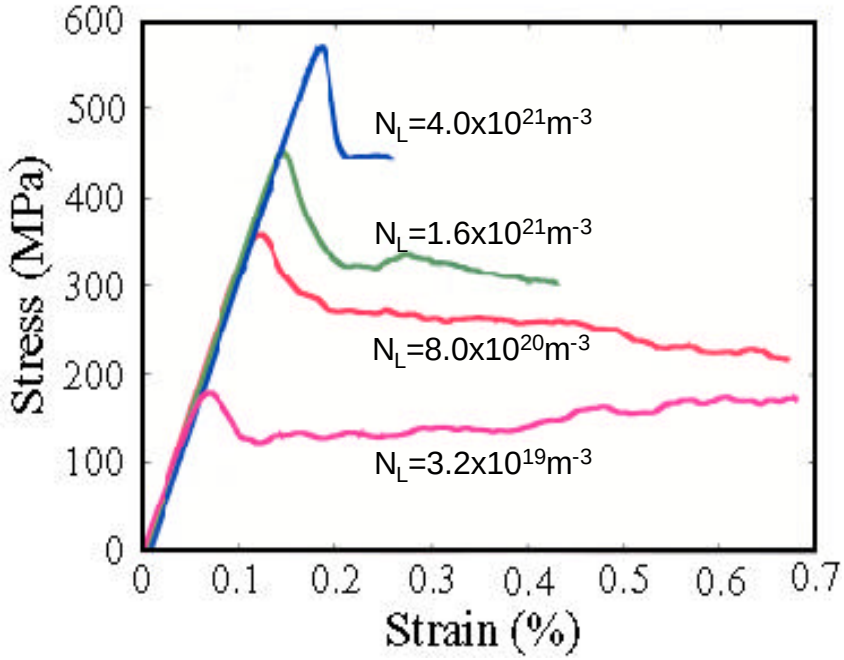
  - Add Stresses

$$s = mb\left(\sqrt{a\,r} + \sqrt{bN_l d_l}\right)$$

Recent Accomplishments: Dislocation Dynamics Simulations Predict the Strength of Irradiated Crystals

- Dislocation Dynamics simulations reveal the origins of irradiation induced strengthening and enable the testing of functional dependencies on irradiation induced defect morphologies





Conclusion

- Nuclear fuel system design is currently an empirical process with long lead times due to test reactor residence times
- Nuclear fuel certifications have typically have narrow operational windows because of a lack of understanding of the system performance and response
- Modeling and Simulation on High Performance Computers has the potential to substantially change the nuclear materials certification and fuel licensing processes
  - Heroic reference calculations can test assumptions built into design codes
  - High throughput design simulations can tackle real fuel geometries
  - Sub-scale physics simulations can discover underlying mechanism controlling materials performance
  - Methods are needed to credibly translate prototypical testing observations into reactor performance predictions